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ERDEC-TR-225

SOME NEW SATURATED TWO-LEVEL DESIGNS



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RESEARCH AND TECHNOLOGY DIRECTORATE

January 1995

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
<small>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</small>				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 1995 January	3. REPORT TYPE AND DATES COVERED Final, 94 Apr - 94 Oct		
4. TITLE AND SUBTITLE Some New Saturated Two-Level Designs		5. FUNDING NUMBERS PR-10161102A71A		
6. AUTHOR(S) Crosier, Ronald B.				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) DIR, ERDEC, ATTN: SCBRD-RTM, APG, MD 21010-5423		8. PERFORMING ORGANIZATION REPORT NUMBER ERDEC-TR-225		
9. SPONSORING MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSORING MONITORING AGENCY REPORT NUMBER		
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) First-order saturated designs can have the two desirable properties of being an orthogonal design and having two levels only if $n \equiv 0 \pmod{4}$, where n is the number of design points. For other cases, researchers have developed D-optimal two level designs. Recently, two-level saturated designs that are efficient for submodels containing only a few of the factors were developed. These p-efficient designs (p is the number of parameters in a submodel) have two properties not possessed by the D-optimal designs: (near) equal-occurrence of -1's and 1's in each column and near orthogonality of each pair of columns. In this report saturated, two-level designs that estimate the effects of all factors with equal precision are developed. These equal-precision designs are generally better than the p-efficient designs by the three criteria D-efficiency, G-efficiency, and maximum variance inflation factor. Equal-precision designs are given for $n=3-30, 38, 42$, and 50.				
14. SUBJECT TERMS Plackett and Burman design Saturated design		15. NUMBER OF PAGES 17		
		16. PRICE CODE		
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

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PREFACE

The work described in this report was authorized under Project No. 10161102A71A, Research in Chemical Weapons/Chemical Biological Defense. This work was started in April 1994 and completed in October 1994.

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SOME NEW SATURATED TWO-LEVEL DESIGNS

1. INTRODUCTION

In many experiments the goal is to determine which of many independent variables (or experimental factors) x_1, x_2, \dots, x_v have the largest effects on the dependent variable y . A common strategy for such problems is to approximate the relationship between y and the process factors by the first-order polynomial

$$y = \beta_0 + \sum_{j=1}^v \beta_j x_j + \epsilon, \quad (1)$$

where the random error ϵ has mean zero and variance σ^2 . The coefficients of the polynomial (1) are estimated from data collected during n experimental runs of the process; the settings of the x 's for the n experimental runs are given by the $n \times v$ design matrix D . To estimate the coefficients of the polynomial, the design matrix is expanded into a model matrix X that has an additional column which represents the constant term. The estimate b of the coefficient vector is then obtained from the least-squares formula

$$b = (X'X)^{-1} X'y. \quad (2)$$

The two-level designs of Plackett and Burman (1946) are widely used to estimate the coefficients in (1). These designs are saturated designs because they estimate the effects of v variables using $n = v + 1$ design points (experimental runs). The Plackett and Burman (1946) designs are only available, however, for $n \equiv 0 \pmod{4}$. The usual strategy when $v + 1$ is not a multiple of 4 is to use the next larger Plackett and Burman design by ignoring 1, 2, or 3 design columns. There are times when one wishes to minimize the number of experimental runs for cases where $v + 1 \not\equiv 0 \pmod{4}$. Much of the work that has been done for such cases has been too theoretical to receive widespread use. For example, the designs were developed to maximize a

single design criterion—the determinant of $X'X$. Lin (1993) reviewed this theoretical work, and proposed some practical properties that such designs should have. Lin (1993) then developed some designs that had those properties. I discuss design properties and criteria for comparing designs in Section 2. In Section 3, I propose two methods for finding two-level saturated designs. Sections 4, 5, and 6 present new saturated two-level designs for the cases $n \equiv 2 \pmod{4}$, $n \equiv 1 \pmod{4}$, and $n \equiv 3 \pmod{4}$, respectively, and compare the designs to Lin's (1993) designs.

2. DESIGN CRITERIA

The D-efficiency of a design for estimating p parameters is the p th root of the ratio of $\det(X'X)/n^p$ to the maximum possible value of $\det(X'X)/n^p$ for any design covering the same region. For two-level saturated designs where the levels are coded -1 and 1 , this definition reduces to

$$D\text{-eff.} = [\det(X'X)]^{1/n}/n. \quad (3)$$

The G-efficiency of a design is defined as $p/V(x)_{\max}$, where p is the number of parameters in the model and $V(x)_{\max}$ is the maximum value of $V(x) = n x'(X'X)^{-1}x$ for any point x in the experimental region. The variance of \hat{y} at x is $V(x)\sigma^2/n$, so the G-efficiency of a design compares the maximum value of $V(x) = n \text{Var}[\hat{y} | x]/\sigma^2$ within the experimental region to its theoretical minimum, which is p . For saturated designs, the formula for G-efficiency becomes

$$G\text{-eff.} = 1/x'(X'X)^{-1}x \quad (4)$$

where x is the point of maximum prediction variance. G-efficiency is a more sensitive criterion than D-efficiency: a design can have a high D-efficiency and a low G-efficiency, but not vice versa. Generally, the point of maximum prediction variance is found at the boundary of the experimental region. In this report, I consider the region of the saturated two-level designs to be a sphere of radius $v^{1/2}$. This choice is well founded because an orthogonal first-order design is also a rotatable design—meaning that the prediction variance is constant on the surface of a sphere centered at the design origin. An orthogonal first-order design has a G-efficiency of 1 over a

spherical region. In a sense, the G-efficiency measures the extent to which a first-order design deviates from orthogonality. G-efficiency could be criticized as a criterion for our two-level designs if the maximum prediction variance occurred at a point like $(v^{1/2}, 0, 0, \dots, 0)$, but in no case did this happen. The worst G-efficiencies in this report are for Lin's (1993) designs for $n \equiv 3 \pmod{4}$; for those designs the point of maximum prediction variance is actually at a vertex of the cube. Hence, for those designs, it makes no difference if the experimental region is considered to be a sphere, a cube, or the vertices of the cube (as would be appropriate if the factors were discrete).

Another measure that can be used to judge the deviation of a first-order design from orthogonality is the maximum variance inflation factor. A variance inflation factor (VIF) measures how much the variance of an estimated coefficient in the model has been inflated by the nonorthogonality of the design. The variances of the estimated coefficients are given by σ^2 times the diagonal elements of $(X'X)^{-1}$. If a two-level design with levels -1 and 1 is orthogonal, the variance of the estimated coefficients is σ^2/n . Hence the variances of the estimated coefficients are inflated by n times the diagonal elements of $(X'X)^{-1}$. When the VIF's for the estimated coefficients are not all the same, the largest VIF is taken as a measure of the nonorthogonality of the design.

Following previous theoretical work, Lin (1993) considered only the D-efficiency of designs. He did, however, restrict his search for designs by requiring that the designs have some properties of practical importance. First, he required that, for even n , there be the same number of 1's and -1's in each column and, for odd n , the number of 1's and -1's differ by only 1. He called this requirement (near) equal-occurrence. He also put limits on the absolute size of s_{ij} , the sum of cross products between columns i and j of the design matrix; he referred to this property as near orthogonality. Lin's (1993) motivation for selecting designs with these properties was to find designs that are efficient for submodels containing only a few of the factors. However, I believe that the efficiency for submodels must be secondary to the efficiency for the full model. Further, for both Lin's (1993) designs and the new designs in this report, submodels for a few factors tend to have higher efficiencies than the full model, so the concern over the efficiencies of submodels does not seem warranted.

A property that I would use in selecting a design for application is that of equal precision—by which I mean that the variances of the estimated

coefficients (except for the constant term) are all equal. Saturated two-level designs are used in situations in which many factors are believed to influence the response y , but it is not known which factors have large effects and which factors have effects small enough to be ignored. The analysis of the data from the designed experiment is essentially to rank the factors from most important to least important. The ranking may be done either by $|b_j|$, or by $|b_j|/c_j$, where c_j is the square root of the diagonal element of $(X'X)^{-1}$ corresponding to x_j . The first method ranks the factors by the absolute size of their effects on the response y , the second by a quantity proportional to the t -test for the significance of the factor. When the c_j (or, equivalently, the VIF's) are all the same, the β_j are all estimated with equal precision, and the ranking of the factors is unambiguous.

3. DESIGN CONSTRUCTION

Lin (1993) generated designs by starting with a randomly selected column and appending, by a computer search algorithm, additional columns so that the designs will have the near orthogonality property; all columns must have the (near) equal-occurrence property. By examining the Plackett and Burman (1946) designs, I developed two methods of generating saturated two-level designs. The Plackett and Burman designs for $n \leq 24$ are obtained by cyclically permuting the first row, and then appending a row of -1 's. One can use this technique for $n \neq 0 \pmod{4}$, by trying all 2^v combinations of -1 's and 1 's for the first row, forming the design by adding the cyclic permutations and a row of -1 's, then rejecting those designs that do not have the (near) equal-occurrence and near orthogonality properties. (This brute force algorithm can be improved in several ways, but the improvements will not be discussed in this report.) One must then calculate the efficiencies of the designs to select the best design; it is possible for a cyclic design having the (near) equal-occurrence and near orthogonality properties to be singular. (This phenomenon shows the weakness of using the size of the s_{ij} —which are the individual elements of $X'X$ —to judge the nonorthogonality of the design.)

The Plackett and Burman (1946) designs are related to balanced incomplete block (BIB) designs. For example, consider the Plackett-Burman design for $n = 8$, whose first row is 1, 1, 1, -1 , 1, -1 , -1 . The location of the 1 's (1, 2, 3, 5) indicate the treatments in the first block of a cyclic BIB design

($v = b = 7$, $r = k = 4$) and the location of the -1 's (4, 6, 7) indicate a block of the complementary cyclic BIB design ($v = b = 7$, $r = k = 3$). [The first block of the design for $k = 3$ is usually written as (1, 2, 4), which can be obtained by reading the first row of the Plackett-Burman design backwards (from right to left); every cyclic pattern works both forwards and backwards.] For $n \not\equiv 0 \pmod{4}$, we will have to use partially balanced incomplete block (PBIB) designs to construct saturated, two-level designs. The treatments in the blocks of the PBIB design will indicate the location of the -1 's in the first v rows; the last row will be all -1 's. The PBIB designs must have $v = b$ and $r = k$; r must be chosen so that the saturated designs have the (near) equal-occurrence property. One can calculate the s_{ij} 's directly from the λ 's of the PBIB design. If i and j are u th associates, then $s_{ij} = b - 4r + 4\lambda_u + 1$. Lin (1993) discusses the possible values for s_{ij} . For $n \equiv 2 \pmod{4}$, I required that $|s_{ij}|$ take its minimum possible value, 2. For n odd, I required that the s_{ij} be -3 and 1 , or -1 and 3 ; it is generally not possible to obtain the absolute value of both s_{ij} 's equal to 1 . For $n \equiv 2 \pmod{4}$, I was able to find (or easily construct) PBIB designs that give satisfactory saturated designs up to $n = 50$, with the exceptions of $n = 34$ and $n = 46$. For odd n , very few PBIB designs with the required parameters were available, so the technique of trying all cyclic patterns was used to construct saturated designs.

4. DESIGNS FOR $n \equiv 2 \pmod{4}$

Table 1 compares Lin's (1993) designs and the PBIB-based designs for $n \equiv 2 \pmod{4}$ by their D- and G-efficiencies and by their VIF's. Lin (1993) did not give his design for $n = 30$, so I was not able to find its G-efficiency or its maximum VIF. The only designs of Lin's (1993) for even n that have the equal-precision property are his designs for $n = 14$ and $n = 26$; those designs are isomorphic to the PBIB-based designs. (Lin's design for $n = 30$ cannot be isomorphic to the PBIB-based design because the average value of s_{ij}^2 , which was reported by Lin (1993), is different for the two designs.) The PBIB-based designs are equal to or better than Lin's (1993) designs by the three criteria D-efficiency, G-efficiency, and VIF; the PBIB-based designs also have the equal-precision property in all cases. The patterns for the cyclic PBIB-based designs (along with other cyclic patterns) are given in Table 2. For the case $n = 10$, there is a cyclic-type saturated design that may be preferred to the PBIB-based design of Table 1. The cyclic design has a D-efficiency of .866, a G-efficiency of .426, and a VIF of 1.37 for all terms (except the constant term)

Table 1. Comparison of Designs for $n \equiv 2 \pmod{4}$.

n	v	Lin's Designs			PBIB-based Designs			
		D-eff.	G-eff.	VIF	D-eff.	G-eff.	VIF	type
6	5	.763	.170	3.00 ^a	.763	.291	2.00	cyclic
10	9	.815	.294	1.71 ^a	.837	.426	1.50	L_2
14	13	.876	.503	1.33	.876	.503	1.33	cyclic
18	17	.891	.280	1.43 ^a	.901	.556	1.25	cyclic
22	21	.858	.115	3.32 ^a	.934	.736	1.14	triangular
26	25	.929	.625	1.17	.929	.625	1.17	L_3
30	29	.938	?	?	.938	.649	1.14	cyclic
38	37				.950	.686	1.11	cyclic
42	41				.955	.700	1.10	cyclic
50	49				.962	.724	1.08	L_4

^a Maximum variance inflation factor.

of the first-order model. The pattern for the cyclic design is given in Table 2.

The triangular PBIB design required for the case $n = 22$ is given in Table 3. To obtain the saturated, two-level design assign a -1 to the variables listed in a block and a 1 to the remaining variables and append a final row of -1 's.

PBIB designs of the Latin square type are denoted as L_2 if they are based on the rows and columns of a square; L_3 if they are based on the rows, columns, and Latin letters of a Latin square; and L_4 if they are based on the rows, columns, Latin letters, and Greek letters of a Greco-Latin square. The numbers 1 to v , which represent the treatments, are written into a square (any order may be used). The first associates of a treatment are those treatments which share a row, a column, a Latin letter (if type L_3), or a Greek letter (if type L_4) with the given treatment.

The three Latin square type PBIB designs referred to by Table 1 have the same, simple construction: the treatments in the i th block are the first associates of treatment i . Hence by writing out the first associates of each treatment, we also have the treatments in every block.

Table 2. Patterns for Cyclic Designs.

n	v	Location of -1's in First Row.
3	2	1
5	4	1
6	5	1,5
7	6	1,2,4
9	8	1,2,4
10	9	1,3,4,8
11	10	1-4,7
13	12	1,2,4,6,7
14	13	1,2,5,9,12,13
15	14	1-4,6,10
17	16	1-4,6,9,13
17	16	1-3,5,10,11,15 ($s_{ij} \leq 5$)
18	17	2,3,4,6,12,14,15,16
19	18	1-4,6,7,10,12,14
21	20	1-5,8,11,13,17
22	21	1-5,7,10,11,15,17
23	22	1-5,9,10,12,15,19
25	24	1-6,9,12,14,16,21,22
26	25	1-5,7,8,11,16,18,20,21
27	26	1-6,10,15,17,20,21,23
29	28	1-5,10,14,15,17,21,24,25,27
30	29	1,3-5,7,12,13,17,18,23,25-27,29
38	37	1,2,4-6,11,13,14,17,21,24,25,27,32-34,36,37
42	41	1,3,5,11-13,16,17,19,20,22,23,25,26,29-31,37,39,41

Cyclically permute the first row to make v rows; append a row of -1's.

The L_4 type PBIB design for the $n = 50$ case requires a 7×7 Greco-Latin square. To make a 7×7 Greco-Latin square, place the Latin letters on diagonals from upper right to lower left [so that the other treatments that share the same Latin letter with a given treatment are found by repeatedly going down 1 row and left 1 column from the given treatment, cycling back to the top or to the right when necessary]; then the other treatments that share the same Greek letter can be found by going down 1 row and left 2 columns, cycling back to the top or to the right when necessary.

Table 3. Triangular PBIB Design

Block	Treatments in Block									
1	2	3	4	5	7	8	11	12	16	17
2	1	3	4	6	7	9	11	13	16	18
3	1	2	5	6	8	9	12	13	17	18
4	1	2	5	6	7	10	11	14	16	19
5	1	3	4	6	8	10	12	14	17	19
6	2	3	4	5	9	10	13	14	18	19
7	1	2	4	8	9	10	11	15	16	20
8	1	3	5	7	9	10	12	15	17	20
9	2	3	6	7	8	10	13	15	18	20
10	4	5	6	7	8	9	14	15	19	20
11	1	2	4	7	12	13	14	15	16	21
12	1	3	5	8	11	13	14	15	17	21
13	2	3	6	9	11	12	14	15	18	21
14	4	5	6	10	11	12	13	15	19	21
15	7	8	9	10	11	12	13	14	20	21
16	1	2	4	7	11	17	18	19	20	21
17	1	3	5	8	12	16	18	19	20	21
18	2	3	6	9	13	16	17	19	20	21
19	4	5	6	10	14	16	17	18	20	21
20	7	8	9	10	15	16	17	18	19	21
21	11	12	13	14	15	16	17	18	19	20

5. DESIGNS FOR $n \equiv 1 \pmod{4}$

With the exception of $n = 13$, designs isomorphic to Lin's (1993) designs for $n \equiv 1$ can be obtained by appending a row and a column to a Plackett and Burman (1946) design; Lin gives row vectors \mathbf{r} and column vectors \mathbf{q}' in his Table 1. The row vectors for $n = 17$ and $n = 21$ in Lin's Table 1 are incorrect; both the row and column vectors for $n = 25$ and $n = 29$ are also incorrect. Using $m(1)$ to indicate m occurrences of 1, the correct row vector for $n = 17$ is 2(1), 8(-1), 1, -1, 3(1); for $n = 21$ the correct \mathbf{r} is 4(1), 10(-1), 5(1). For $n = 25$, $\mathbf{r} = 2(1), 3(-1), 1, -1, 1, 9(-1), 2(1), -1, 3(1)$ and $\mathbf{q}' = 4(-1), 2(1), 6(-1), 1, -1, 10(1)$. For $n = 29$, $\mathbf{r} = 6(1), 2(-1), 1, 3(-1), 2(1), -1, 1, -1, 2(1), 2(-1), 3(1), 2(-1), 1$ and $\mathbf{q}' = 4(1), 3(-1), 3(1), -1, 4(1), -1, 1, -1, 2(1), -1, 1, 6(-1)$.

Table 4 compares Lin's (1993) designs for $n \equiv 1 \pmod{4}$ to some new designs obtained by trying cyclic patterns.

Table 4. Comparison of Designs for $n \equiv 1 \pmod{4}$.

n	v	Lin's Designs			Cyclic-based Designs		
		D-eff.	G-eff.	VIF	D-eff.	G-eff.	VIF
5	4	.941	.800	1.11	.941	.800	1.11
9	8	.932	.472	1.47 ^a	.888	.471	1.32
13	12	.977	.923	1.04	.876	.324	1.43
17	16	.954	.400	1.68 ^a	.919	.246	1.24
17	16				.904	.525	1.21 ^b
21	20	.963	.406	1.68 ^a	.939	.465	1.15
25	24	.969	.424	1.65 ^a	.937	.466	1.16
29	28	.974	.450	1.61 ^a	.956	.538	1.10

^a Maximum variance inflation factor.

^b This alternative design has some $s_{ij} = 5$.

Of Lin's designs for $n \equiv 1 \pmod{4}$, only those for $n = 5$ and $n = 13$ have the equal-precision property; designs formed by a cyclic pattern and a row of -1 's always have the equal-precision property. Lin's design for $n = 5$ and the cyclic design are the same design. Lin's design for $n = 13$ is very good; it has $X'X = (n-1)I_n + J_n$, where I_n is an $n \times n$ identity matrix and J_n is an $n \times n$ matrix of 1 's. That pattern for $X'X$ is only possible if $2n-1$ is the square of an integer. Lin's design for $n = 13$ can be obtained from the PBIB design denoted SR41 in the catalog of Clatworthy (1973). As usual, the treatments in a block of the design (Table 5) indicate the locations of the -1 's in the first b rows. The PBIB design SR41 has $b = 9$, but we need $n = 13$ rows, so four extra rows must be added (instead of the usual row of -1 's). In the four added rows, three variables corresponding to a group of first associates are assigned 1 's and the remaining nine variables are assigned -1 's. The four groups of first associates are (1, 5, 9), (2, 6, 10), (3, 7, 11), and (4, 8, 12).

Two cyclic designs are given for $n = 17$. The first was the result of the usual search where all $|s_{ij}|$ are required to be less than or equal to 3. The resulting design was not appealing because of its low G-efficiency, so another search, allowing $|s_{ij}|$ to be as large as 5 was tried. The first design has 24

Table 5. PBIB Design SR41

Block	Treatments in the Block			
1	1	2	3	4
2	1	6	7	8
3	1	10	11	12
4	2	5	8	11
5	2	7	9	12
6	3	5	6	12
7	3	8	9	10
8	4	5	7	10
9	4	6	9	11

$s_{ij} = -3$ and 96 $s_{ij} = 1$; the second design has 32 $s_{ij} = -3$, 80 $s_{ij} = 1$, and 8 $s_{ij} = 5$. Clearly the second design is worse by the $ave(s_{ij}^2)$ criterion used by Lin (1993), but it may be preferred because of its better G-efficiency and lower VIF.

6. DESIGNS FOR $n \equiv 3 \pmod{4}$

Lin's (1993) designs for $n \equiv 3 \pmod{4}$ are obtained by deleting a row and a column from a Plackett and Burman (1946) design. It does not matter which row and column are deleted; the resulting designs are isomorphic. However, by deleting the last row, the designs have $X'X = (n+1)I_n - J_n$. Lin (1993) found that the D-efficiency of these designs is $(n+1)^{(n-1)/n}/n$, which is a monotonically increasing function of n ; however, a more thorough evaluation of the designs would have discovered that their G-efficiency is $1/n$, which is a monotonically decreasing function of n . Thus the pattern $(n+1)I_n - J_n$ for $X'X$ is seen to be undesirable, despite having low correlations between pairs of variables.

Table 6 compares Lin's designs for $n \equiv 3 \pmod{4}$ to some designs obtained from cyclic patterns. Lin's design for $n = 3$ and the cyclic design are isomorphic. The cyclic design for $n = 7$ is a cyclic PBIB design [it is also a regular group divisible PBIB design; Clatworthy (1973) lists it as R42].

Table 6. Comparison of Designs for $n \equiv 3 \pmod{4}$.

n	v	Lin's Designs			Cyclic-based Designs		
		D-eff.	G-eff.	VIF	D-eff.	G-eff.	VIF
3	2	.840	.333	1.50	.840	.333	1.50
7	6	.849	.143	1.75	.878	.571	1.30
11	10	.870	.091	1.83	.890	.384	1.30
15	14	.887	.067	1.88	.910	.483	1.21
19	18	.899	.053	1.90	.940	.640	1.13
23	22	.909	.043	1.92	.946	.624	1.11
27	26	.917	.037	1.93	.949	.601	1.11

Attempts to find designs with higher G-efficiencies for the cases $n = 11$ and $n = 15$ by allowing the values of $|s_{ij}|$ to be as large as 5 did not succeed. Although Lin's designs for $n \equiv 3 \pmod{4}$ have the equal-precision property, they will probably not be used because of their low G-efficiencies.

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